August 2004

Final Report Summary: December 2003 Peer Review of the CMAQ Model

Introduction

The external CMAQ Model Program Peer Review Panel that reviewed the CMAQ model in December 2003 provides this report in order to assess the current state of the model, to guide its development in the short term, and to assess the appropriateness of resources (institutional support, staffing, and operational funding) in the long term to achieve desired advances. The report is written from the range of perspectives represented by the seven members of the review panel:

- Praveen Amar (Northeast States for Coordinated Air Use Management)
- Robert Bornstein (San Jose State University)
- Howard Feldman (American Petroleum Institute)
- Harvey Jeffries (The University of North Carolina at Chapel Hill)
- Douw Steyn (The University of British Columbia)
- Robert Yamartino (consultant, Integrals Unlimited)
- Yang Zhang (North Carolina State University)

The panel members read a considerable volume of material on CMAQ provided by EPA, and attended two days of presentations on CMAQ by EPA staff.

Federal, state, and local governments as well as regional organizations have used 3-D deterministic models such as CMAQ with one fundamental goal in mind: evaluation and the optimum selection of alternative control strategies to attain ambient standards for various criteria pollutants. The main regulatory purpose of such models is to understand how future changes in emissions ("delta E") would result in future changes in concentrations of various pollutants ("delta C"). Ozone (1-h standard) has been the primary focus so far, and fine particles (those below 2.5 μm and/or 10 μm in diameter) will be the new focus in addition to a continuing focus on ozone (8-h standard). From the science, policy, and implementation perspectives, particulate matter (PM) will be much more challenging than ozone, in that PM has an annual standard (in addition to the 24-h standard) that requires annual modeling (unlike ozone, which is usually modeled over periods of a few days to a few weeks). Also, our present understanding of PM chemistry and physics is considerably weaker than that for ozone, though the understanding of PM is evolving rapidly. PM modeling has additional problems related to the need for acceptable and quality-assured annual data for emissions, and atmospheric measurements for model evaluation. In addition, the most sophisticated treatments of aerosol chemistry and physics will lead to substantial increases in computational requirements (run time and hardware requirements).

The CMAQ model must take into account the fact that ozone plus PM modeling could involve considerably more than twice the work of ozone modeling alone. Also, in addition to ozone and

PM, it is important for CMAQ to address the issues of air toxics (including mercury) and acid deposition.

These considerations provided a context for the panel's review of CMAQ. Of great interest and concern are efforts to expand the range of the model's scales of applicability into both the micro scale (through "urbanization" of its 1-km-scale version) and the global scale. Such scale expansion, while consistent with a growing trend toward "end-to-end" models, presents considerable technical and computational challenges, made more challenging when faced with limited resources.

CMAQ is a massive computer code designed to model a wide range of physical and chemical processes that occur at particular scales in the lower atmosphere. Some of these processes are well understood (for example, dispersion of pollutants by mean wind and turbulent fluctuations), some processes reasonably well understood (for example, the production of oxidant substances by photochemical reactions between volatile organic substances and oxides of nitrogen), and some processes only poorly understood (for example, the production of organic nitrate aerosols by heterogeneous reactions between volatile organic substances and oxides of nitrogen). This range of knowledge about the processes being modeled, and the fact that processes subject to uncertainty are the subject of active research worldwide, means that parts of the model code are well-established enough to be considered fixed, while other parts of the code are in constant development. The result of this is that there must exist at all times two versions of the model: (1) a currently active, reasonably stable version of CMAQ that is used in an operational and regulatory mode, and, in parallel, (2) a development version of CMAQ that is continually being improved by the CMAQ development team. From time to time, the development version replaces the operational version, thus bringing recent advances in atmospheric science to the operational realm. Having a model exist in both operational and research realms is a situation not uncommon for computer codes. However, the existence of these two versions considerably complicates the task of this review panel. The panel concentrated its attention on the operational version of CMAQ, but where appropriate, has referred in this report to characteristics of the development version. Clearly the development version is closer to "state of the science" than is the operational version, and the differences are most marked in areas that are topics of current research.

The main substance of this report is thus a review and set of recommendations designed to assess the current state of CMAQ and to guide its development in the short term. These statements are primarily directed at the operational version of CMAQ. As requested by EPA, the panel concentrated on five areas of interest:

1. What is the overall quality of the scientific research in the CMAQ Modeling Program?
2. What are the strengths and weaknesses of the science being used within the components of the CMAQ Model development program?
3. What is the quality and relevance of the research applications and model evaluations being conducted as part of the CMAQ Modeling Program?
4. What are your perceptions of the integration across the elements of the CMAQ Modeling Program (links between model development, applications, evaluation)? What is your

perception of the usefulness of the CMAQ Modeling Program to the EPA and ORD Agency mission?

5. Are there modeling research areas that are not being addressed or are given insufficient attention within the CMAQ Modeling Program? Are there current areas of research emphasis that might be given lower priority or eliminated? For the resources available to the CMAQ Modeling Program, are they being used in an effective manner in terms of the choice and quality of research being conducted?

Panel Report

This panel report is presented as a set of recommendations. These are not ranked in order of priority, but are grouped merely for convenience.

Overall Recommendations

- The CMAQ effort should remain focused on its main mission. From the perspective of its major clients, this is urban/regional modeling of PM and ozone for State Implementation Plan (SIP) purposes. The main regulatory purpose of CMAQ and similar models is to provide an understanding of how future changes in emissions would result in future changes in concentrations of various pollutants.

- The core research effort of the CMAQ modeling program should focus on model improvements and urban/regional applications. The research effort in air quality modeling at a fine scale and up to a global scale to study the linkages among air quality, health impacts, and global change is important, but should not distract from the main effort of developing CMAQ as an urban- to regional-scale model.

- We believe that air quality forecasting is an important and worthwhile goal that could be accomplished with CMAQ, supplemented with other less intensive tools such as Auto-regression Integrated Moving Average (ARIMA) or Artificial Neural Net (ANN) statistical models. Since long-term air quality forecasting (>1 month) may provide potentially important information for SIPs, EPA should coordinate their efforts and resources effectively with the lead organizations charged with achieving this capability, such as the National Oceanic and Atmospheric Administration (NOAA) and National Center for Atmospheric Research (NCAR).

Core Model Capability and Applicability

- We recommend that enhancing the chemical and dynamic aspects of PM modeling in CMAQ become a top priority. We note that the primary objective of the Atmospheric Modeling Division's (AMD's) CMAQ model research program is to develop **operational air quality models** for use by EPA and the states in making emission management decisions. A continuing focus of scientific improvement should be on CMAQ's aerosol treatments. Much effort has gone into improving these treatments over the past several years, but there remains room for improvement. It is also important to note that while CMAQ is a leader in this area among other operational air quality models, all such models lag noticeably behind worldwide research efforts.

- We recommend that EPA maintain its position in the forefront of model evaluation for the types of applications for which CMAQ is used. Operational evaluation should be expanded into more insightful diagnostic/mechanistic/probabilistic evaluation. A guideline/protocol for PM evaluation should be published by EPA.

- We recommend that the CMAQ team perform an in-house evaluation of emissions modeling by use of techniques such as "inverse modeling."

Fine-Scale and Global-Scale Model Applicability

- We recommend that EPA and others undertake an investigation of the range of scales (temporal and spatial) over which the model can legitimately be applied. Results of this investigation should be publicized to all users.

- Recognizing pressure from users and regulators to provide a nested modeling capability down to the scale of urban canyons, we recommend EPA move cautiously in this logical next step, given the significant challenges on the meteorological side of developing a linkage of the Pennsylvania State University/NCAR Mesoscale Model (version 5) (MM5) to computational fluid dynamics (CFD) and/or large eddy simulation (LES) codes.

Air Quality Forecasting

- We recommend that EPA resist pressures to implement nesting within the Weather Research and Forecasting model (WRF), as we believe that this task should be undertaken by NCAR. We note also that WRF will have to incorporate nudging capability for it to be an appropriate driver for CMAQ, but such data assimilation capabilities are also demanded by weather forecasters. Thus, EPA should also not be responsible for implementing nudging, but should work to ensure that this capability is included into WRF in a manner well-suited to both weather forecasters and air quality modelers.

- We recommend that EPA coordinate efforts and resources effectively with other organizations (e.g., NOAA, NCAR) to develop a version of CMAQ for real-time operational forecasting that leads to development of a nationwide air quality forecasting program.

CMAQ User and Developer Communities

- Recent key staff retirements in the ORD CMAQ group raise concern about continuation of the PM modeling effort. Given the importance of PM modeling to EPA's mandate in the $PM_{2.5}$-PM_{10} areas and given the complexity of aerosol physics and chemistry, we recommend that the modeling group work actively to ensure they have sufficient research-level staff to support needed PM modeling efforts.

- We recommend that the CMAQ model development team increase its number of postdoctoral researchers, as these personnel will be most likely to introduce continuing improvements into CMAQ.

- We recommend that EPA, or others, develop a group of beta testers who will test research and operational (pre-released) versions of CMAQ, while the current released version is in active use.

- We recommend that EPA widely and publicly acknowledge the contributions of non-EPA developers and beta testers of CMAQ. This should include those providing code extensions, modifications, corrections, and bug fixes. A mechanism to implement bug fixes discovered in this way should be established.

- We recommend that EPA staff be given time and resources to build collaborative links to non-EPA researchers, so as to ensure that CMAQ reflects the state of the science in all its aspects. This could be achieved through focused workshops or conferences on topics central to the development of CMAQ.

- We recommend the creation of a mechanism for the periodic review of CMAQ to ensure that it remains state of the science. We strongly recommend that the scientific review of CMAQ be made an ongoing activity and be undertaken about every two years.

- We recommend that the CMAQ team carefully consider efforts underway to improve MM5, so as to avoid working in problem areas that parallel the efforts of the meteorological community. This will free staff to work on problem areas that are "CMAQ-specific."

- We support EPA's current and quite successful efforts in its outreach to scientific and regulatory communities through CMAS. It is extremely important that CMAS have sufficient public and private resources to offer focused training classes and workshops relating to various components of CMAQ.